

# 3D Visualization of Chemical Transport in Porous Media

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## **3D VISUALIZATION OF CHEMICAL TRANSPORT IN POROUS MEDIA**

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### **ABSTRACT**

Chemical transport in porous media has been studied experimentally via a novel nonintrusive fluorescence imaging technique. The technique involves 3D visualization and quantification of chemical concentration fields within a refractive index-matched transparent porous system. The system consists of a porous column packed with spherical beads and a refractive index-matched fluid flowing through the column at a steady state. A fluorescent organic dye is steadily introduced into the flow at the bottom of the column and allowed to migrate through the medium. The refractive index-matching yields a transparent porous medium, free from any scattering and refraction at the solid-liquid interfaces, as a result allowing direct optical probing at any point within the porous system. By illuminating the flow within the column with a planar sheet of laser beam, chemical transport through the porous medium can be observed microscopically, and qualitative and quantitative in-pore transport information can be obtained at a good resolution. A CCD camera is used to record the fluorescent images at every vertical plane location while sweeping back and forth across the column. These images are then analyzed and accumulated over a 3D volume within the column. Three-dimensional concentration fields have been determined successfully within the system. This paper reports on 3D observations of chemical

concentration changes with time at the pore-scale level within the porous medium.

### **INTRODUCTION**

The present paper reports on an experimental effort to improve our understanding of chemical/contaminant transport in soils and other porous media by investigating the transport at the microscopic spatial scale.

Previous experimental investigations (Harleman and Rumer 1963, Hassinger and Von Rosenberg 1968, Klotz et al. 1980, and Han et al. 1985) have provided some valuable information on the macroscopic behavior of the flow and transport in porous media. Even though, many bulk transport phenomena result from the flow behavior at the microscopic spatial scale, until recently, little work has been done on the microscopic characterization of processes at the pore-scale. This can be attributed to the experimental difficulty of nonintrusively measuring flow and transport at high resolutions within the solid matrix. Recent experimental improvements have allowed some investigations of pore-scale processes. These include studies using certain forms of noninvasive optical techniques (PIV, NMRI) in and above packed beds for velocity and porosity measurements (Stephenson and Stewart 1986, Bories et al. 1991, Saleh et al. 1993, Li et al. 1994, and Derbyshire et al. 1994) and studies in surrogate media composed of two-dimensional etched glass or capillary network

micromodels (Soll et al. 1993, Soll and Celia 1993, and Wan and Wilson 1994).

Theoretical descriptions of flow and transport in porous media have been generally derived from simpler "bulk" equations of mass and momentum balance or from more systematic approaches in which pore-scale behavior is rigorously averaged over representative elementary volume (REV) of the medium. The works of Whitaker (1967, 1969), Slattery (1967, 1972), Bear (1972), Gray (1975), Hassanizadeh and Gray (1983), and Gray et al. (1993) are representative of the current approach in this field. While each model presents a slightly different point of view, all require some assumptions about a specific medium behavior that must be confirmed and parameterized by detailed experimental work.

The present work is part of an extensive research in our laboratory to understand the microscopic transport processes within porous media (Peurrung et al. 1995). We have developed a novel nonintrusive imaging technique to observe pore-scale behavior at a high resolution and a high accuracy. The paper presents some of the interstitial concentration results obtained using our technique. The overall objective is to use these results and future findings toward understanding of chemical transport through a porous medium and, as a result, provide the basis for realistic modeling of chemical/contaminant transport in natural or commercial porous systems.

## EXPERIMENTAL FACILITIES

Figure 1 shows the detail of experimental setup and measurement techniques. Experiments were performed in a clear polymethylmethacrylate (PMMA) cylindrical packed column 4.5 cm in diameter and about 23.5 cm in length. The column was filled uniformly with PMMA spherical beads of 3.1 mm. A mixture of silicone oils (Dow Corning 550 and 556) was chosen as the fluid which matched the beads' refractive index of 1.4885 at 19.8°C and a wavelength of 514.5 nm. The column was maintained at this temperature throughout all runs by being immersed in a circulating constant temperature bath. A syringe pump was used to provide a constant volumetric flow rate of the above fluid at 1.15 cm<sup>3</sup>/min.

The experiments were done with the refractive matched fluid seeded with an organic fluorescent dye for concentration measurements. The column was illuminated by an Argon-ion laser (coherent)

operated at 475 nm for velocity measurements and 488 nm for concentration measurements. A CCD camera was used to record the experimental runs. Since, the dye emission peaks around 514.5 nm, a band pass filter was used on the video camera to pass a narrow range of 514.5 nm  $\pm$  5 nm wavelength associated with the dye excitation. The video camera was placed perpendicular to the laser propagation beam on a remotely operated platform such that it moved with the beam in order to scan various cross-section of the column.

The refractive index-matching yielded a transparent porous medium, free from any scattering and refraction at the solid-liquid interfaces, thus allowing direct optical probing at any point within the porous system. In these experiments, a neutrally buoyant dye was steadily introduced into the column and its concentration was imaged by sequentially scanning the concentration fields in vertical cross-sections. The video camera recorded fluorescence images at every vertical plane location while sweeping back and forth (with the illumination plane) across the column at every minute.

The experimental runs were recorded through the video camera by a computer controlled VCR (Sony, EVO-9650) in Hi-8 mm format. The VCR was a frame accurate model that produced high quality still images of specified frames. It was computer controlled through an RS-232 interface for automated concentration analysis. In order to capture the recorded images for data analysis, a frame grabber board (ITI PC Vision Plus) with 640 by 480 pixel resolution was used in conjunction with an IBM compatible 486-33 computer. The image analysis was done using the OPTIMAS (BioScan) software. Several detailed programs were developed as interface softwares for automated experimental run and analysis softwares for concentration measurements. In order to evaluate the uncertainty in the measurements a test run was performed. The uncertainty in the values of concentration was about 5% at 95% confidence level for 200 frames analyzed (see Rashidi and Banerjee 1988).

## RESULTS

Experiments were carried out, in which a dye front was injected into the porous system for concentration measurements. Experimental data were collected over a three-dimensional volume within the column by scanning the illumination

plane across that region. As previously described, the camera and laser sheet were placed on a platform that moved back and forth at a controlled speed for scanning the column. During the experiment which lasted about 120 minutes, up to 60,000 individual measurement points of concentration were collected each minute (corresponding to 22 vertical slices). This resulted in an enormous amount of experimental data within the porous medium. The collected data were later placed in three dimensional arrays that could be presented in a 3D fashion.

As shown in Figure 2, once these sliced results are assembled into volumetric arrays, the data can be sampled in various ways to determine different attributes of the overall flow field. Figure 3 shows 3D plots of concentration distributions as a function of time within the porous medium. Here, the values of concentrations are nondimensionalized by the saturated concentration values and the flow direction is from bottom to top. Furthermore, smaller values of concentration (less than 0.1) are masked out in order to show the high concentrated regions. As seen in this figure, the porous medium becomes saturated as the experiment continues and the detail of transport phenomena can be observed dynamically. These plots show the enormous amount of chemical transport information that can be derived from the microscopically measured data. This information can be used to derive sound theoretical transport models or to check the prediction of the existing transport models.

## CONCLUSIONS

Chemical transport in porous media has been visualized and measured microscopically using a unique nonintrusive fluorescence imaging technique. The test section consists of a porous column packed with spherical beads and a refractive index-matched fluid. The system is automated to image through the porous medium for collecting microscopic values of concentration. Experiments were carried out in which a dye front was injected into the porous system and its dispersion was tracked. Concentration values were obtained in a full three-dimensional volume of the test section at a good accuracy and a high resolution of up to 60,000 measurement points for a given time. These measurements show the dynamic detail of transport processes within porous geometries as the system becomes saturated.

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## REFERENCES

- Bear, J., 1972, "Dynamics of Fluids in Porous Media," Elsevier, New York, NY.
- Bories, S.A., Charrier-Mojtabi, M.C., Houi, D. and Raynaud, P.G., 1991, "Noninvasive measurement techniques in porous media," *Convective Heat and Mass Transfer in Porous Media*, S. Kakac et al. (eds.), Kluwer Academic Publishers, Netherlands.
- Derbyshire, J.A., Gibbs, S.J., Carpenter, T.A. and Hall, L.D., 1994, "Rapid three-dimensional velocimetry by Nuclear Magnetic Resonance imaging," *AIChE J.* **40**, 1404-1407.
- Gray, W.G., 1975, "A derivation of the equations for multi-phase transport," *Chem. Engng Sci.* **30**, 229-233.
- Gray, W. G., Leijnse, A., Kolar, R.L. and Blain, C.A., 1993, "Mathematical Tools of Changing Spatial Scales in the Analysis of Physical Systems," CRC Press, Boca Raton.
- Han, N.W., Bhakta, J. and Carbonell, R.G., 1985, "Longitudinal and lateral dispersion in packed beds: Effect of column length and particle size distribution," *AIChE J.* **31**, 277-288.
- Harleman, D.R.E. and Rumer, R.R., 1963, "Longitudinal and lateral dispersion in an isotopic porous medium," *J. Fluid Mech.* **16**, 385-394.
- Hassanizadeh, S.M. and Gray, W.G., 1979, "General conservation equations for multi-phase systems: Averaging procedures," *Advances in Water Resources* **2**, 131-144.
- Hassinger, R.C. and Von Rosenberg, D.U., 1968, "A mathematical and experimental examination of transverse dispersion coefficients," *Trans. Soc. Pet. Eng. J.* **243**, 195-204.
- Klotz, D., Seiler, K.P., Moser, H. and Neumaier, F., 1980, "Dispersivity and velocity relationship from laboratory and field experiments," *J. Hydrol.* **45**, 169-184.
- Li, T., Seymour, J.D., Powell, R.L., McCarthy, M.J., MacCarthy, K.L. and Ödberg, L., 1994, "Visualization of flow patterns of cellulose fiber

suspensions by NMR imaging," *AIChE J.* **40**, 1408-1411.

Peurrung, L., Rashidi, M., and Kulp, T.J., 1994, "Measurement of porous medium velocity fields and their volumetric averaging characteristics using particle tracking velocimetry," *Chem. Engng Sci.* (accepted).

Rashidi, M. and Banerjee, S., 1988, "Turbulence structure in free surface channel flows," *Phys. Fluids* **31**, 2491-2503.

Saleh, S., Thovert, J.F. and Adler, P.M., 1993, "Flow along porous media by particle image velocimetry," *AIChE J.* **39**, 1765-1776.

Slattery, J.C., 1967, "Flow of viscoelastic fluids through porous media," *AIChE J.* **13**, 1066-1071.

Slattery, J.C., 1972, "Momentum, Energy, and Mass Transfer in Continua," McGraw-Hill, New York, NY.

Soll, W.E., Celia, M.A. and Wilson, J.L., 1993, "Micromodel studies of three-fluid porous media systems: Pore-scale processes relating to capillary pressure-saturation relationships," *Water Resour. Res.* **29**, 2963-2974.

Soll, W. E. and Celia, M.A., 1993, "A modified percolation approach to simulating 3-fluid capillary pressure saturation relationships," *Adv. Wat. Resour.*, **16** (2), 107-126.

Stephenson, J.L. and Stewart, W.E., 1986, "Optical measurements of porosity and fluid motion in packed beds," *Chem. Eng. Sci.* **41**, 2161-2170.

Wan, J. and Wilson, J.L., 1994, "Visualization of the role of the gas-water interface on the fate and transport of collids in porous media," *Water Resour. Res.* **30**, 11-23.

Whitaker, S., 1967, "Diffusion and dispersion in porous media," *AIChE J.* **13**, 420-429.

Whitaker, S., 1969, "Advances in theory of fluid motion in porous media," *Ind. Eng. Chem.* **61**, 14-28.

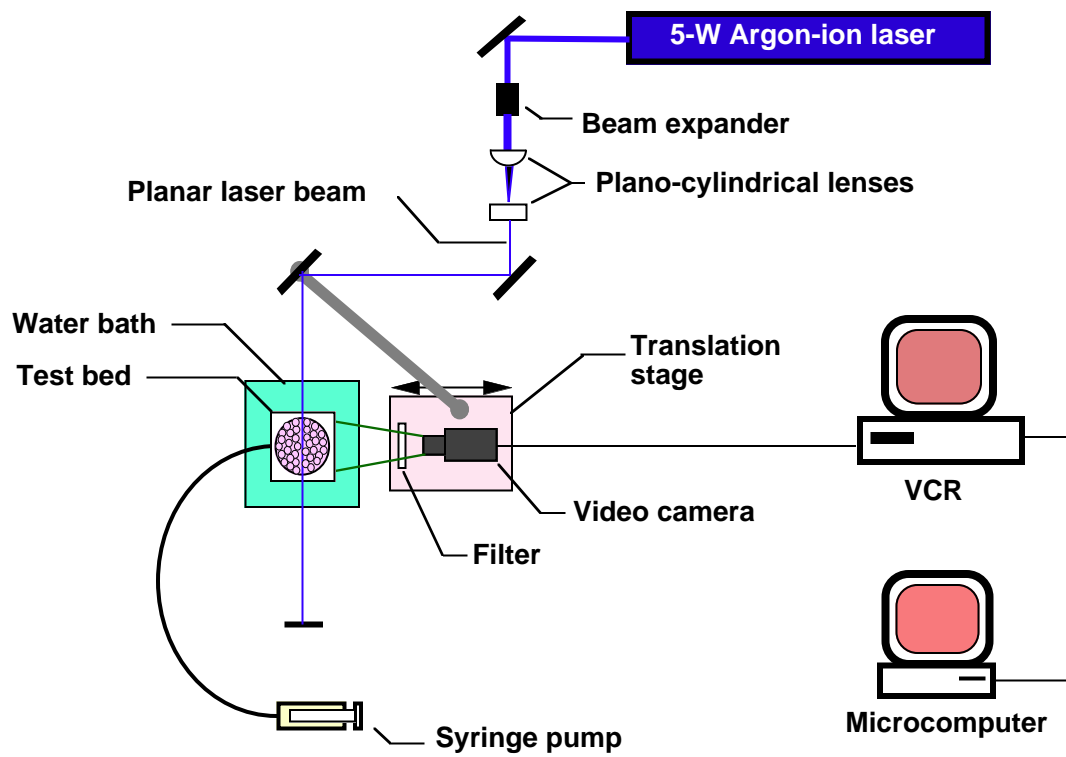


Figure 1. Experimental setup and measurement apparatus.

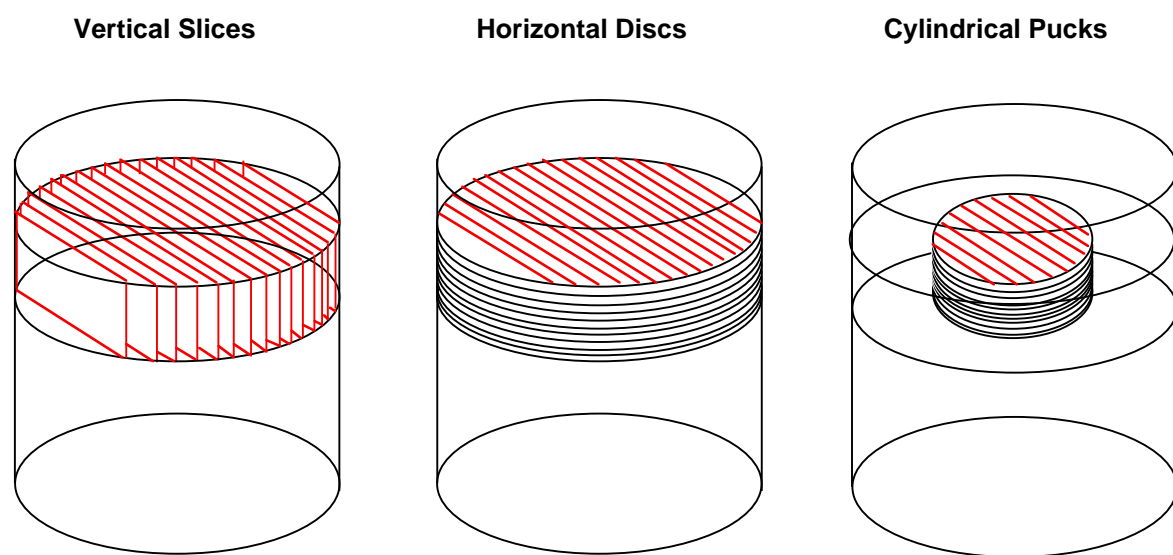


Figure 2. Data representation in form of vertical slices, horizontal discs, and cylindrical pucks of varying radius.



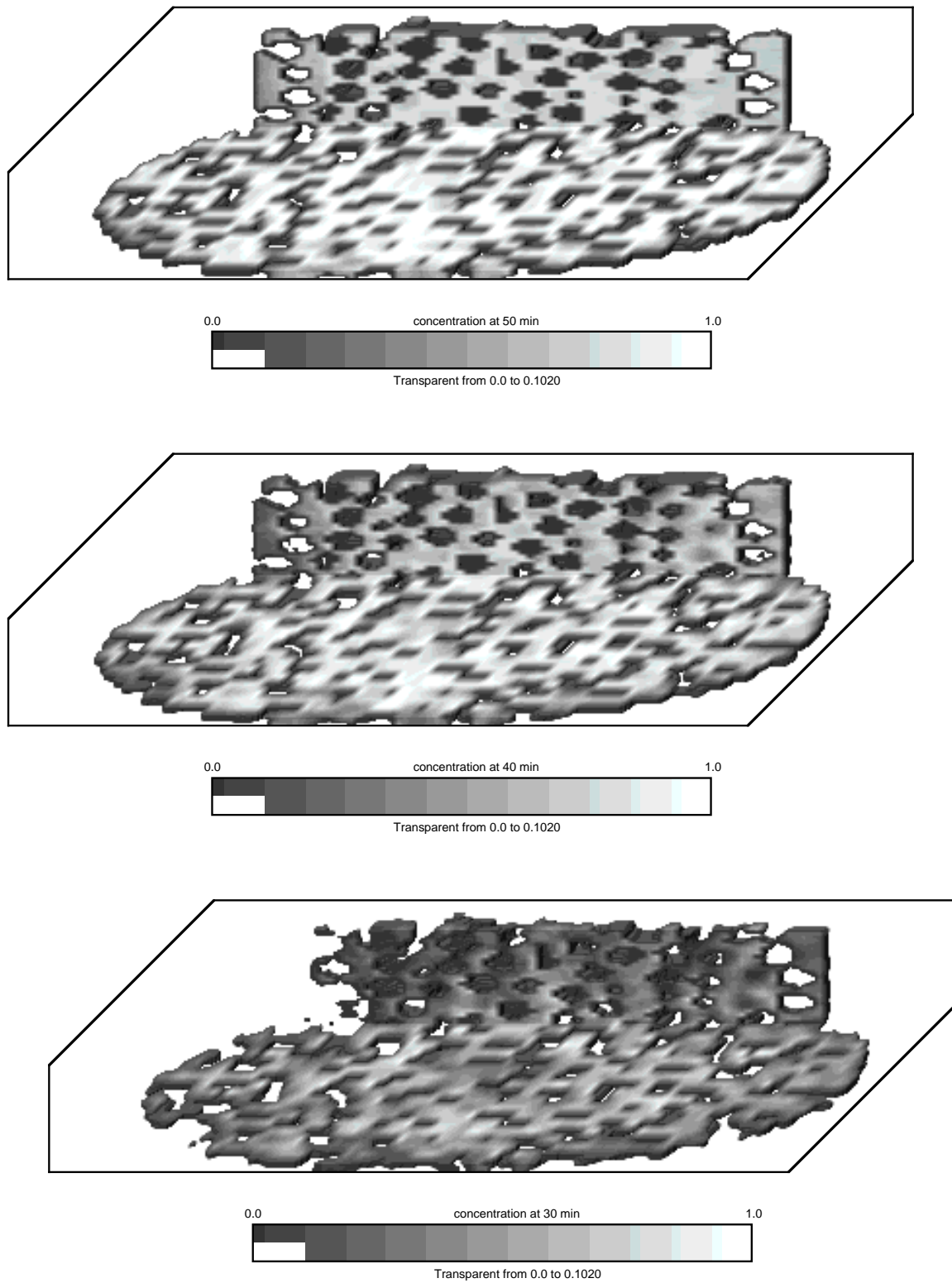


Figure 3. 3D plots of non-dimensionalized concentration distributions as a function of time in the porous medium. Here, smaller values of concentrations are masked out at each time. Flow direction is from bottom to top and concentrations are non-dimensionalized by saturated concentration values.





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